

Containment, Equivalence and Coreness from CSP to QCSP and beyond.

Barnaby Martin

Engineering and Computing Sciences, Durham University, U.K.*

barnabymartin@gmail.com

Florent Madelaine

Clermont Université, Université d'Auvergne,
Clermont-Ferrand, France.

florent.madelaine@googlemail.com

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Abstract

The constraint satisfaction problem (CSP) and its quantified extensions, whether without (QCSP) or with disjunction (QCSP_∨), correspond naturally to the model checking problem for three increasingly stronger fragments of positive first-order logic. Their complexity is often studied when parameterised by a fixed model, the so-called template. It is a natural question to ask when two templates are equivalent, or more generally when one “contain” another, in the sense that a satisfied instance of the first will be necessarily satisfied in the second. One can also ask for a smallest possible equivalent template: this is known as the core for CSP. We recall and extend previous results on containment, equivalence and “coreness” for QCSP_∨ before initiating a preliminary study of cores for QCSP which we characterise for certain structures and which turns out to be more elusive.

1 Introduction

We consider the following increasingly stronger fragments of first-order logic:

1. primitive positive first-order ($\{\exists, \wedge\}$ -FO)
2. positive Horn ($\{\exists, \forall, \wedge\}$ -FO)
3. positive equality-free first-order ($\{\exists, \forall, \wedge, \vee\}$ -FO); and,
4. positive first-order logic ($\{\exists, \forall, \wedge, \vee, =\}$ -FO)

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The *model checking problem* for a logic \mathcal{L} takes as input a sentence of \mathcal{L} and a structure \mathcal{B} and asks whether \mathcal{B} models \mathcal{L} . The structure \mathcal{B} is often assumed to be a fixed parameter and called the template; and, unless otherwise stated, we will assume implicitly that we work in this so-called *non-uniform* setting.

For the above first three fragments, the model checking problem is better known as the *constraint satisfaction problem* $\text{CSP}(\mathcal{B})$, the *quantified constraint satisfaction problem* $\text{QCSP}(\mathcal{B})$ and its extension with disjunction which we shall denote by $\text{QCSP}_\vee(\mathcal{B})$. Much of the theoretical research into CSPs is in respect of a large complexity classification project – it is conjectured that $\text{CSP}(\mathcal{B})$ is always either in P or NP-complete [9]. This *dichotomy* conjecture remains unsettled, although dichotomy is now known on substantial classes (e.g. structures of size ≤ 3 [16, 3] and smooth digraphs [11, 1]). Various methods, combinatorial (graph-theoretic), logical and universal-algebraic have been brought to bear on this classification project, with many remarkable consequences. A conjectured delineation for the dichotomy was given in the algebraic language in [4].

Complexity classifications for QCSPs appear to be harder than for CSPs. Just as $\text{CSP}(\mathcal{B})$ is always in NP, so $\text{QCSP}(\mathcal{B})$ is always in Pspace. No overarching polychotomy has been conjectured for the complexities of $\text{QCSP}(\mathcal{B})$, as \mathcal{B} ranges over finite structures, but the only known complexities are P, NP-complete and Pspace-complete (see [2, 15] for some trichotomies). It seems plausible that these complexities are the only ones that can be so obtained.

Distinct templates may give rise to the same model-checking-problem or preserve acceptance,

(\mathcal{L} -**equivalence**) for any sentence φ of \mathcal{L} , \mathcal{A} models $\varphi \Leftrightarrow \mathcal{B}$ models φ

(\mathcal{L} -**containment**) for any sentence φ of \mathcal{L} , \mathcal{A} models $\varphi \Rightarrow \mathcal{B}$ models φ .

We will see that containment and therefore equivalence is decidable, and often quite effectively so, for the four logics we have introduced.

For example, when \mathcal{L} is $\{\exists, \wedge\}$ -FO, any two bipartite undirected graphs that have at least one edge are equivalent. Moreover, there is a canonical *minimal* representative for each equivalence class, the so-called *core*. For example, the core of the class of bipartite undirected graphs that have at least one edge is the graph \mathcal{K}_2 that consists of a single edge. The core enjoys many benign properties and has greatly facilitated the classification project for CSPs (which corresponds to the model-checking for $\{\exists, \wedge\}$ -FO): it is unique up to isomorphism and sits as an induced substructure in all templates in its equivalence class. A core may be defined as a structure all of whose endomorphisms are automorphisms. To review, therefore, it is well-known that two templates \mathcal{A} and \mathcal{B} are equivalent iff there are homomorphisms from \mathcal{A} to \mathcal{B} and from \mathcal{B} to \mathcal{A} , and in this case there is an (up to isomorphism) unique core \mathcal{C} equivalent to both \mathcal{A} and \mathcal{B} such that $\mathcal{C} \subseteq \mathcal{A}$ and $\mathcal{C} \subseteq \mathcal{B}$.

The situation for $\{\exists, \forall, \wedge\}$ -FO and QCSP is somewhat murkier. It is known that non-trivial \mathcal{A} and \mathcal{B} are equivalent iff there exist integers r and r' and surjective homomorphisms from \mathcal{A}^r to \mathcal{B} and from $\mathcal{B}^{r'}$ to \mathcal{A} (and one may give a bound on these exponents) [6]. However, the status and properties of “core-ness” for QCSP were hitherto unstudied.

We **might** call a structure \mathcal{B} a *Q-core* if there is no equivalent \mathcal{A} of strictly smaller cardinality. We will discover that **this** Q-core is a more cumbersome beast than its cousin the core; it need not be unique nor sit as an induced substructure of the templates in its class. However, in many cases we shall see that its behaviour is reasonable and that – like the core – it can be very useful in delineating complexity classifications.

The erratic behaviour of Q-cores sits in contrast not just to that of cores, but also that of the U - X -cores of [13], which are the canonical representatives of the equivalence classes associated with $\{\exists, \forall, \wedge, \vee\}$ -FO, and were instrumental in deriving a full complexity classification – a tetrachotomy – for QCSP_\vee in [13]. Like cores, they are unique and sit as induced substructures in all templates in their class. Thus, primitive positive logic and positive equality-free logic behave genially in comparison to their wilder cousin positive Horn. In fact this manifests on the algebraic side also – polymorphisms and surjective hyper-endomorphisms are stable under composition, while surjective polymorphisms are not.

Continuing to add to our logics, in restoring equality, we might arrive at positive logic. Two finite structures agree on all sentences of positive logic iff they are isomorphic – so here every finite structure satisfies the ideal of “core”. When computing a/the smallest substructure with the same behaviour with respect to the four decreasingly weaker logics – positive logic, positive equality-free, positive Horn, and primitive positive – we will obtain possibly decreasingly smaller structures. In the case of positive equality-free and primitive positive logic, as pointed out, these are unique up to isomorphism; and for the U - X -core and the core, these will be induced substructures. A Q-core will necessarily contain the core and be included in the U - X -core. This phenomenon is illustrated on Table 1 and will serve as our running example.

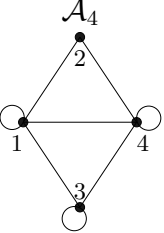
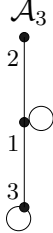


$\{\exists, \forall, \wedge, \vee, =\}$ -FO	$\{\exists, \forall, \wedge, \vee\}$ -FO	$\{\exists, \forall, \wedge\}$ -FO	$\{\exists, \wedge\}$ -FO
			
isomorphism	U - X -Core	Q-core	Core

Table 1: Different notions of “core” (the circles represent self-loops).

The paper is organised as follows. In Section 2, we recall folklore results on CSP. In Section 3, we recall results on coreness and spell out containment for $\{\exists, \forall, \wedge, \vee\}$ -FO that were only implicit in [13]. In Section 4, we move on to QCSP and recall results on the decidability of containment from [6] together with new lower bounds before initiating a study of the notion of core for QCSP .

2 The case of CSP

Unless otherwise stated, we consider structures over a fixed relational signature σ . We denote by A the domain of a structure \mathcal{A} and for every relation symbol R in σ of arity r , we write $R^{\mathcal{A}}$ for the interpretation of R in \mathcal{A} , which is a r -ary relation that is $R^{\mathcal{A}} \subseteq A^r$. We write $|A|$ to denote the cardinality of the set A . A homomorphism (resp., strong homomorphism) from a structure \mathcal{A} to a structure \mathcal{B} is a function $h : A \rightarrow B$ such that $(h(a_1), \dots, h(a_r)) \in R^{\mathcal{B}}$, if (resp., iff) $(a_1, \dots, a_r) \in R^{\mathcal{A}}$.

We will occasionally consider signatures with constant symbols. We write $c^{\mathcal{A}}$ for the interpretation of a constant symbol c and homomorphisms are required to preserve constants as well, that is $h(c^{\mathcal{A}}) = c^{\mathcal{B}}$.

Containment for $\{\exists, \wedge\}$ -FO is a special case of conjunctive query containment from databases [5]. We state and prove these results for pedagogical reasons, before moving to the case of $\{\exists, \forall, \wedge, \vee\}$ -FO. Let us fix some notation first. Given a sentence φ in $\{\exists, \wedge\}$ -FO, we denote by \mathcal{D}_φ its *canonical database*, that is the structure with domain the variables of φ and whose tuples are precisely those that are atoms of φ . In the other direction, given a finite structure \mathcal{A} , we write $\varphi_{\mathcal{A}}$ for the so-called *canonical conjunctive query* of \mathcal{A} , the quantifier-free formula that is the conjunction of the positive facts of \mathcal{A} , where the variables $v_1, \dots, v_{|\mathcal{A}|}$ correspond to the elements $a_1, \dots, a_{|\mathcal{A}|}$ of \mathcal{A} .¹ It is well known that there is a homomorphism from \mathcal{D}_φ to a structure \mathcal{A} if, and only if, $\mathcal{A} \models \varphi$. Moreover, a winning strategy for \exists in the (Hintikka) (\mathcal{A}, φ) -game is precisely a homomorphism from \mathcal{D}_φ to \mathcal{A} . Note also that \mathcal{A} is isomorphic to the canonical database of $\exists v_1 \exists v_2 \dots v_{|\mathcal{A}|} \varphi_{\mathcal{A}}$.

Theorem 1 (Containment). *Let \mathcal{A} and \mathcal{B} be two structures. The following are equivalent.*

- (i) *for every sentence φ in $\{\exists, \wedge\}$ -FO, if $\mathcal{A} \models \varphi$ then $\mathcal{B} \models \varphi$.*
- (ii) *There exists a homomorphism from \mathcal{A} to \mathcal{B} .*
- (iii) *$\mathcal{B} \models \exists v_1 \exists v_2 \dots v_{|\mathcal{A}|} \varphi_{\mathcal{A}}$.*

where $\varphi_{\mathcal{A}}$ denotes the canonical conjunctive query of \mathcal{A} .

Proof. A homomorphism corresponds precisely to a winning strategy in the (\mathcal{A}, φ) -game and (ii) and (iii) are equivalent. Clearly, (i) implies (iii) since $\mathcal{A} \models \exists v_1 \exists v_2 \dots v_{|\mathcal{A}|} \varphi_{\mathcal{A}}$.

We now prove that (ii) implies (i). Let h be a homomorphism from \mathcal{A} to \mathcal{B} . If $\mathcal{A} \models \varphi$, then there is a homomorphism g from \mathcal{D}_φ to \mathcal{A} . By composition, $g \circ h$ is a homomorphism from \mathcal{D}_φ to \mathcal{B} . In other words, $g \circ h$ is a winning strategy witnessing that $\mathcal{B} \models \varphi$. \square

It is well known that the core is unique up to isomorphism and that it is an induced substructure [12]. It is usually defined via homomorphic equivalence, but because of the equivalence between (i) and (ii) in the above theorem, we may define the core as follows.

Definition 1. *The core \mathcal{B} of a structure \mathcal{A} is a minimal substructure of \mathcal{A} such that for every sentence φ in $\{\exists, \wedge\}$ -FO, $\mathcal{A} \models \varphi$ if and only if $\mathcal{B} \models \varphi$.*

Corollary 1 (equivalence). *Let \mathcal{A} and \mathcal{B} be two structures. The following are equivalent.*

- (i) *for every sentence φ in $\{\exists, \wedge\}$ -FO, $\mathcal{A} \models \varphi$ if and only if $\mathcal{B} \models \varphi$.*
- (ii) *There are homomorphisms from \mathcal{A} to \mathcal{B} and from \mathcal{B} to \mathcal{A} .*
- (iii) *The core of \mathcal{A} and the core of \mathcal{B} are isomorphic.*

As a preprocessing step, one could replace the template \mathcal{A} of a CSP by its core \mathcal{B} (see Algorithm 6.1 in [7]). However, the complexity of this preprocessing step would be of the same order of magnitude as solving a constraint satisfaction problem.² This drawback, together with the uniform nature of the instance in constraints solvers, means that this preprocessing is not exploited in practice to the best of our knowledge.

The notion of a core can be extended and adapted suitably to solve important questions related to data exchange and query rewriting in databases [8]. It is also very useful as a simplifying assumption when classifying the complexity: with the algebraic approach, it allows to study only idempotent algebras [4].

¹Most authors consider the canonical query to be the sentence which is the existential quantification of $\varphi_{\mathcal{A}}$.

²Checking that a graph is a core is coNP-complete [10]. Checking that a graph is the core of another given graph is DP-complete [8].

3 The case of QCSP with disjunction

For $\{\exists, \forall, \wedge, \vee\}$ -FO, it is no longer the homomorphism that is the correct concept to transfer winning strategies.

Definition 2. A surjective hypermorphism f from a structure \mathcal{A} to a structure \mathcal{B} is a function from the domain A of \mathcal{A} to the power set of the domain B of \mathcal{B} that satisfies the following properties.

- (**total**) for any a in A , $f(a) \neq \emptyset$.
- (**surjective**) for any b in B , there exists a in A such that $f(a) \ni b$.
- (**preserving**) if $R(a_1, \dots, a_i)$ holds in \mathcal{A} then $R(b_1, \dots, b_i)$ holds in \mathcal{B} , for all $b_1 \in f(a_1), \dots, b_i \in f(a_i)$.

A strategy for \exists in the (Hintikka) (\mathcal{A}, φ) -game, where $\varphi \in \{\exists, \forall, \wedge, \vee\}$ -FO, is a set of mappings $\{\sigma_x : ' \exists x' \in \varphi\}$ with one mapping σ_x for each existentially quantified variable x of φ . The mapping σ_x ranges over the domain A of \mathcal{A} ; and, its domain is the set of functions from Y_x to A , where Y_x denotes the universally quantified variables of φ preceding x .

We say that $\{\sigma_x : ' \exists x' \in \varphi\}$ is *winning* if for any assignment π of the universally quantified variables of φ to A , when each existentially quantified variable x is set according to σ_x applied to $\pi|_{Y_x}$, then the quantifier-free part ψ of φ is satisfied under this overall assignment h . When ψ is disjunction-free, this amounts to h being a homomorphism from \mathcal{D}_ψ to \mathcal{A} .

Lemma 1 (strategy transfer). Let \mathcal{A} and \mathcal{B} be two structures such that there is a surjective hypermorphism from \mathcal{A} to \mathcal{B} . Then, for every sentence φ in $\{\exists, \forall, \wedge, \vee\}$ -FO, if $\mathcal{A} \models \varphi$ then $\mathcal{B} \models \varphi$.

Proof. Let f be a surjective hypermorphism from \mathcal{A} to \mathcal{B} and φ be a sentence of $\{\exists, \forall, \wedge, \vee\}$ -FO such that $\mathcal{A} \models \varphi$. For any element b of \mathcal{B} , let $f^{-1}(b) := \{a \in A \text{ s. t. } b \in f(a)\}$. We fix an arbitrary linear order over A and write $\min f^{-1}(b)$ to denote the smallest antecedent of b in A under f .

Let $\{\sigma_x : ' \exists x' \in \varphi\}$ be a winning strategy in the (\mathcal{A}, φ) -game. We construct a strategy $\{\sigma'_x : ' \exists x' \in \varphi\}$ in the (\mathcal{B}, φ) -game as follows. Let $\pi_B : Y_x \rightarrow B$ be an assignment to the universal variables Y_x preceding an existential variable x in φ , we select for $\sigma'_x(\pi)$ an arbitrary element of $f(\sigma(\pi_A))$ where $\pi_A : Y_x \rightarrow A$ is an assignment such that for any universal variable y preceding x , we have $\pi_A(y) := \min f^{-1}(\pi_B(y))$. This strategy is well defined since f is surjective (which means that π_A is well defined) and total (which means that $f(\sigma(\pi_A)) \neq \emptyset$). Note moreover that using \min in the definition of π_A means that a branch in the tree of the game on \mathcal{B} will correspond to a branch in the tree of the game on \mathcal{A} . It remains to prove that $\{\sigma'_x : ' \exists x' \in \varphi\}$ is winning. We will see that it follows from the fact that f is preserving.

Assume first that φ is a sentence of $\{\exists, \forall, \wedge\}$ -FO. Let \mathcal{D}_ψ be the canonical database of the quantifier-free part ψ of φ . The winning condition of the (\mathcal{B}, φ) -game can be recast as a homomorphism from \mathcal{D}_ψ . Composing with f the homomorphism from \mathcal{D}_ψ to \mathcal{A} (induced by the sequence of compatible assignments π_A to the universal variables and the strategy $\{\sigma_x : ' \exists x' \in \varphi\}$), we get a surjective hypermorphism from \mathcal{D}_ψ to \mathcal{B} . The map from the domain of \mathcal{D}_ψ to \mathcal{B} induced by the sequence of assignments π_B and the strategy $\{\sigma'_x : ' \exists x' \in \varphi\}$ is a range restriction of this surjective hypermorphism and is therefore a homomorphism (we identify surjective hypermorphism to singletons with homomorphisms).

When φ is not a sentence of $\{\exists, \forall, \wedge\}$ -FO, we write its quantifier-free part in disjunctive normal form as a disjunction of conjunctions-of-atoms ψ_i . The winning condition can now be recast as a homomorphism from some \mathcal{D}_{ψ_i} . The above argument applies and the result follows. \square

Example 1. Consider the structures \mathcal{A}_4 and \mathcal{A}_3 from Table 1. The map f given by $f(1) := \{1\}, f(2) := \{2\}, f(3) := \{3\}, f(4) := \{1\}$ is a surjective hypermorphism from \mathcal{A}_4 to \mathcal{A}_3 . The map g given by $g(1) := \{1, 4\}, g(2) := \{2\}, g(3) := \{3\}$ is a surjective hypermorphism from \mathcal{A}_3 to \mathcal{A}_4 . The two templates are equivalent w.r.t. $\{\exists, \forall, \wedge, \vee\}$ -FO.

We extend the notion of canonical conjunctive query of a structure \mathcal{A} . Given a tuple of (not necessarily distinct) elements $\mathbf{r} := (r_1, \dots, r_l) \in A^l$, define the quantifier-free formula $\varphi_{\mathcal{A}(\mathbf{r})}(v_1, \dots, v_l)$ to be the conjunction of the positive facts of \mathbf{r} , where the variables v_1, \dots, v_l correspond to the elements r_1, \dots, r_l . That is, $R(v_{\lambda_1}, \dots, v_{\lambda_i})$ appears as an atom in $\varphi_{\mathcal{A}(\mathbf{r})}$ iff $R(r_{\lambda_1}, \dots, r_{\lambda_i})$ holds in \mathcal{A} . When \mathbf{r} enumerates the elements of the structure \mathcal{A} , this definition coincides with the usual definition of canonical conjunctive query. Note also that there is a strong homomorphism from the canonical database $\mathcal{D}_{\varphi_{\mathcal{A}(\mathbf{r})}}$ to \mathcal{A} given by the map $r_i \mapsto v_i$.

Definition 3 (Canonical $\{\exists, \forall, \wedge, \vee\}$ -FO sentence). Let \mathcal{A} be a structure and $m > 0$. Let \mathbf{r} be an enumeration of the elements of \mathcal{A} .

$$\theta_{\mathcal{A}, m} := \exists v_1, \dots, v_{|\mathcal{A}|} \varphi_{\mathcal{A}(\mathbf{r})}(v_1, \dots, v_{|\mathcal{A}|}) \wedge \forall w_1, \dots, w_m \bigvee_{\mathbf{t} \in A^m} \varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{v}, \mathbf{w}).$$

Observe that $\mathcal{A} \models \theta_{\mathcal{A}, m}$. Indeed, we may take as witness for the variables \mathbf{v} the corresponding enumeration \mathbf{a} of the elements of \mathcal{A} ; and, for any assignment $\mathbf{t} \in A^m$ to the universal variables \mathbf{w} , it is clear that $\mathcal{A} \models \varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{a}, \mathbf{t})$ holds.

Lemma 2 (strategy transfer). Let \mathcal{A} and \mathcal{B} be two structures. If $\mathcal{B} \models \theta_{\mathcal{A}, |\mathcal{B}|}$ then there is a surjective hypermorphism from \mathcal{A} to \mathcal{B} .

Proof. Let $\mathbf{b}' := b'_1, \dots, b'_{|\mathcal{A}|}$ be witnesses for $v_1, \dots, v_{|\mathcal{A}|}$. Assume that an enumeration $\mathbf{b} := b_1, b_2, \dots, b_{|\mathcal{B}|}$ of the elements of \mathcal{B} is chosen for the universal variables $w_1, \dots, w_{|\mathcal{B}|}$. Let $\mathbf{t} \in A^m$ be the witness s.t. $\mathcal{B} \models \varphi_{\mathcal{A}(\mathbf{r})}(\mathbf{b}') \wedge \varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{b}', \mathbf{b})$.

Let f be the map from the domain of \mathcal{A} to the power set of that of \mathcal{B} which is the union of the following two partial hyperoperations h and g (i.e. $f(a_i) := h(a_i) \cup g(a_i)$ for any element a_i of \mathcal{A}), which guarantee totality and surjectivity, respectively.

- (**totality**) $h(a_i) := b'_i$
- (**surjectivity**) $g(t_i) \ni b_i$.

It remains to show that f is preserving. This follows from $\mathcal{B} \models \varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{b}', \mathbf{b})$.

Let R be a r -ary relational symbol such that $R(a_{i_1}, \dots, a_{i_r})$ holds in \mathcal{A} . Let $b''_{i_1} \in f(a_{i_1}), \dots, b''_{i_r} \in f(a_{i_r})$. We will show that $R(b''_{i_1}, \dots, b''_{i_r})$ holds in \mathcal{B} . Assume for clarity of the exposition and w.l.o.g. that from i_1 to i_k the image is set according to h and from i_{k+1} to i_r according to g : i.e. for $1 \leq j \leq k$, $h(a_{i_j}) = b'_{i_j} = b''_{i_j}$ and for $k+1 \leq j \leq r$, there is some l_j such that $t_{l_j} = a_{i_j}$ and $g(t_{l_j}) \ni b''_{i_j} = b_{l_j}$. By definition of $\mathcal{A}(\mathbf{r}, \mathbf{t})$ the atom $R(v_{i_1}, \dots, v_{i_k}, w_{l_{k+1}}, \dots, w_r)$ appears in $\varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{v}, \mathbf{w})$. It follows from $\mathcal{B} \models \varphi_{\mathcal{A}(\mathbf{r}, \mathbf{t})}(\mathbf{b}', \mathbf{b})$ that $R(b''_{i_1}, \dots, b''_{i_r})$ holds in \mathcal{B} . \square

Theorem 2 (Containment for $\{\exists, \forall, \wedge, \vee\}$ -FO). Let \mathcal{A} and \mathcal{B} be two structures. The following are equivalent.

- (i) for every sentence φ in $\{\exists, \forall, \wedge, \vee\}$ -FO, if $\mathcal{A} \models \varphi$ then $\mathcal{B} \models \varphi$.
- (ii) There exists a surjective hypermorphism from \mathcal{A} to \mathcal{B} .

(iii) $\mathcal{B} \models \theta_{\mathcal{A},|B|}$

where $\theta_{\mathcal{A},\mathcal{B}}$ is a canonical sentence of $\{\exists, \forall, \wedge, \vee\}$ -FO that is defined in terms of \mathcal{A} and $|\mathcal{B}|$ and that is modelled by \mathcal{A} by construction.

Proof. By construction $\mathcal{A} \models \theta_{\mathcal{A},|B|}$, so (i) implies (iii). By Lemma 1, (ii) implies (i). By Lemma 2, (iii) implies (i). \square

Let U and X be two subsets of A and a surjective hypermorphism h from \mathcal{A} to \mathcal{A} that satisfies $h(U) = A$ and $h^{-1}(X) = A$. Let \mathcal{B} be the substructure of \mathcal{A} induced by $B := U \cup X$. Then f and g , the range and domain restriction of h to B , respectively, are surjective hypermorphisms between \mathcal{A} and \mathcal{B} witnessing that \mathcal{A} and \mathcal{B} satisfy the same sentence of $\{\exists, \forall, \wedge, \vee\}$ -FO. Note that in particular h induces a retraction of \mathcal{A} to a subset of X ; and, dually a retraction of the complement structure³ of \mathcal{B} to a subset of U . Additional minimality conditions on U , X and $U \cup X$ ensure that \mathcal{B} is minimal.⁴ It is also *unique* up to isomorphism and within \mathcal{B} the set U and X are *uniquely determined*. Consequently, \mathcal{B} is called **the** U - X -core of \mathcal{A} (for further details see [13]) and may be defined as follows.

Definition 4. *The U - X core \mathcal{B} of a structure \mathcal{A} is a minimal substructure of \mathcal{A} such that for every sentence φ in $\{\exists, \forall, \wedge, \vee\}$ -FO, $\mathcal{A} \models \varphi$ if and only if $\mathcal{B} \models \varphi$.*

Example 2. The map $h(1) := \{1, 4\}, h(2) := \{2\}, h(3) := \{1, 3, 4\}, h(4) := \{1, 4\}$ is a surjective hypermorphism from \mathcal{A}_4 to \mathcal{A}_4 with $U = \{2, 3\}$ and $X := \{1, 2\}$. The substructure induced by $U \cup X$ is \mathcal{A}_3 . It can be checked that it is minimal.

The U - X -core is just like the core an induced substructure. There is one important difference in that U - X -cores should be genuinely viewed as a minimal equivalent substructure induced by *two* sets. Indeed, when evaluating a sentence of $\{\exists, \forall, \wedge, \vee\}$ -FO, we may assume w.l.o.g. that all \forall variables range over U and all \exists variables range over X . This is because for any play of \forall , we may extract a winning strategy for \exists that can even restrict herself to play only on X [13, Lemma 5]. Hence, as a *preprocessing step*, one could compute U and X and restrict the domain of each universal variable to U and the domain of each universal variable to X . *The complexity of this processing step is no longer of the same magnitude* and is in general much lower than solving a QCSP _{\forall} .⁵ Thus, even when taking into account the uniform nature of the instance in a quantified constraints solver, this preprocessing step might be exploited in practice. This could turn out to be ineffective when there are few quantifier alternation (as in bilevel programming), but should be of particular interest when the quantifier alternation increases. Another interesting feature is that storing a winning strategy over U and X together with the surjective hypermorphism h from \mathcal{A} to \mathcal{A} , allows to recover a winning strategy even when \forall plays in an unrestricted manner. This provides a *compression mechanism* to store certificates.

4 The case of QCSP

In primitive positive and positive Horn logic, one normally considers equalities to be permitted. From the perspective of computational complexity of CSP and QCSP, this distinction is unimportant as equalities may be propagated out by substitution. In the case of positive Horn and QCSP,

³It has the same domain as \mathcal{A} and a tuple belongs to a relation R iff it did not in \mathcal{A} .

⁴This is possible since given h_1 s.t. $h_1(U) = A$ and h_2 such that $h_2^{-1}(X) = A$, their composition $h = h_2 \circ h_1$ satisfies both $h(U) = A$ and $h^{-1}(X) = A$.

⁵The question of U - X -core identification is in DP (and should be complete), whereas QCSP _{\forall} is Pspace-complete in general

though, equality does allow the distinction of a trivial case that can not be recognised without it. The sentence $\forall x x = x$ is true exactly on structures of size one. The structures \mathcal{K}_1 and $2\mathcal{K}_1$, containing empty relations over one element and two elements, respectively, are therefore distinguishable in $\{\exists, \forall, \wedge, =\}$ -FO, but not in $\{\exists, \forall, \wedge\}$ -FO. Since we disallow equalities, many results from this section apply only to *non-trivial* structures of size ≥ 2 . Note that equalities can not be substituted out from $\{\exists, \forall, \wedge, \vee, =\}$ -FO, thus it is substantially stronger than $\{\exists, \forall, \wedge, \vee\}$ -FO.

For $\{\exists, \forall, \wedge\}$ -FO, the correct concept to transfer winning strategies is that of *surjective homomorphism from a power*. Recall first that the *product* $\mathcal{A} \times \mathcal{B}$ of two structures \mathcal{A} and \mathcal{B} has domain $\{(x, y) : x \in A, y \in B\}$ and for a relation symbol R , $R^{\mathcal{A} \times \mathcal{B}} := \{((a_1, b_1), \dots, (a_r, b_r)) : (a_1, \dots, a_r) \in R^{\mathcal{A}}, (b_1, \dots, b_r) \in R^{\mathcal{B}}\}$; and, similarly for a constant symbol c , $c^{\mathcal{A} \times \mathcal{B}} := (c^{\mathcal{A}}, c^{\mathcal{B}})$. The *m*th power \mathcal{A}^m of \mathcal{A} is $\mathcal{A} \times \dots \times \mathcal{A}$ (*m* times).

Lemma 3 (strategy transfer). *Let \mathcal{A} and \mathcal{B} be two structures and $m \geq 1$ such that there is a surjective homomorphism from \mathcal{A}^m to \mathcal{B} . Then, for every sentence φ in $\{\exists, \forall, \wedge\}$ -FO, if $\mathcal{A} \models \varphi$ then $\mathcal{B} \models \varphi$.*

Proof. For $m = 1$, the proof is similar to Lemma 1. A projection from \mathcal{A}^m to \mathcal{A} is a surjective homomorphism. This means that for every sentence φ in $\{\exists, \forall, \wedge\}$ -FO, if $\mathcal{A}^m \models \varphi$ then $\mathcal{A} \models \varphi$. For the converse, one can consider the “product strategy” which consists in projecting over each coordinate of \mathcal{A}^m and applying the strategy for \mathcal{A} . For further details see [6, Lemma 1&2]. \square

Example 3. Consider an undirected bipartite graphs with at least one edge \mathcal{G} and \mathcal{K}_2 the graph that consists of a single edge. There is a surjective homomorphism from \mathcal{G} to \mathcal{K}_2 . Note also that $\mathcal{K}_2 \times \mathcal{K}_2 = \mathcal{K}_2 + \mathcal{K}_2$ (where $+$ stands for disjoint union) which we write as $2\mathcal{K}_2$. Thus, $\mathcal{K}_2^j = 2^{j-1}\mathcal{K}_2$ (as \times distributes over $+$). Hence, if \mathcal{G} has no isolated element and m edges there is a surjective homomorphism from $\mathcal{K}_2^{1+\log_2 m}$ to \mathcal{G} .

This examples provides a lower bound for m which we can improve.

Proposition 1 (lower bound). *For any $m \geq 2$, there are structures \mathcal{A} and \mathcal{B} with $|A| = m$ and $|B| = m+1$ such that there is only a surjective homomorphism from \mathcal{A}^j to \mathcal{B} provided that $j \geq |A|$.*

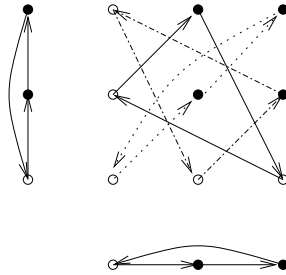


Figure 1: The power of oriented cycles is a sum of oriented cycles.

sketch. We consider a signature that consists of a binary symbol E together with a monadic predicate R . Consider for \mathcal{A} an oriented cycle with m vertices, for which R holds for all but one. Consider for \mathcal{B} an oriented cycle with m vertices, for which R does not hold, together with a self-loop on which R holds. The square of \mathcal{A} will consists of $|A| = m$ oriented cycles with m vertices: one cycle will be a copy of \mathcal{A} , all the other will be similar but with two vertices on which R does not hold (this is depicted on Figure 1 in the case $m = 3$: white vertices do not satisfy R while black ones do). It is only for $j = m$ that we will get as an induced substructure of \mathcal{A}^j one copy of an oriented cycle on which R does not hold as in \mathcal{B} . \square

There is also a *canonical* $\{\exists, \forall, \wedge\}$ -FO-sentence which turns out to be in Π_2 -form, that is with a quantifier prefix of the form $\forall^* \exists^*$. We consider temporarily structures with m constants c_1, c_2, \dots, c_m ; let \mathbf{t} in A^m describe the position of these constants in a structure \mathcal{A} ; and, write $\mathcal{A}_{\mathbf{t}}$ for the corresponding structure with constants. We consider the canonical conjunctive query of the structure with constants $\bigotimes_{\mathbf{t} \in A^m} \mathcal{A}_{\mathbf{t}}$, (where \bigotimes denote the product), identifying the constants with some variables $\mathbf{w} = w_1, \dots, w_m$ and using variables \mathbf{v} for the other elements. We turn this quantifier-free formula into a sentence by adding the prefix $\forall \mathbf{w} \exists \mathbf{v}$. Keeping this in mind, we can also give the following direct definition, but it dilutes the intuition somewhat.

Definition 5 (Canonical $\{\exists, \forall, \wedge\}$ -FO sentence). Let \mathcal{A} be a structure and $m > 0$. Let \mathbf{r} be an enumeration of the elements of $\tilde{\mathcal{A}} := \mathcal{A}^{|A|^m}$.

$$\psi_{\mathcal{A},m} := \forall \mathbf{w} \exists \mathbf{v} \varphi_{\tilde{\mathcal{A}}(\mathbf{r})}(\mathbf{v}) \wedge \bigwedge_{\mathbf{t} \in A^m} w_1 = v_{\mathbf{t},\mathbf{t}[1]} \dots \wedge w_m = v_{\mathbf{t},\mathbf{t}[m]}.$$

Observe that we may propagate the equalities out of $\psi_{\mathcal{A},m}$ to obtain an equivalent sentence: e.g. we remove $w_1 = v_{\mathbf{t},\mathbf{t}[1]}$ and replace every occurrence of $v_{\mathbf{t},\mathbf{t}[1]}$ by w_1 . Observe also that $\mathcal{A} \models \psi_{\mathcal{A},m}$. Indeed, assume that $\mathbf{t} \in A^m$ is the assignment chosen for the universal variables \mathbf{w} . There is a natural projection from $\bigotimes_{\mathbf{t} \in A^m} \mathcal{A}_{\mathbf{t}}$ to $\mathcal{A}_{\mathbf{t}}$ which is a homomorphism. This homomorphism corresponds precisely to a winning strategy for the existential variables \mathbf{v} .

Theorem 3 (Containment for $\{\exists, \forall, \wedge\}$ -FO). Let \mathcal{A} and \mathcal{B} be two non-trivial structures. The following are equivalent.

- (i) for every sentence φ in $\{\exists, \forall, \wedge\}$ -FO, if $\mathcal{A} \models \varphi$ then $\mathcal{B} \models \varphi$.
- (ii) There exists a surjective homomorphism from \mathcal{A}^r to \mathcal{B} , with $r \leq |A|^{|B|}$.
- (iii) $\mathcal{B} \models \psi_{\mathcal{A},|B|}$

where $\psi_{\mathcal{A},|B|}$ is a canonical sentence of $\{\exists, \forall, \wedge\}$ -FO with quantifier prefix $\forall^{|B|} \exists^*$ that is defined in terms of \mathcal{A} and modelled by \mathcal{A} by construction.

sketch. (ii) implies (i) by Lemma 3. (i) implies (iii) since \mathcal{A} models $\psi_{\mathcal{A},|B|}$. (iii) implies (ii) by construction of $\psi_{\mathcal{A},|B|}$. We may chose for the universal variables \mathbf{w} an enumeration of \mathcal{B} . The winning strategy on \mathcal{B} induces a surjective homomorphism from \mathcal{A}^r (for further details see [6, Theorem 3] and comments on the following page). \square

Following our approach for the other logics, we now define a minimal representative as follows.

Definition 6. A Q-core \mathcal{B} of a structure \mathcal{A} is a minimal substructure of \mathcal{A} such that for every sentence φ in $\{\exists, \forall, \wedge\}$ -FO, $\mathcal{A} \models \varphi$ if and only if $\mathcal{B} \models \varphi$.

Example 4. Consider \mathcal{A}_3 and \mathcal{A}_2 from Table 1. The map $f(1) := 1, f(2) := 2, f(3) := 2$ is a surjective homomorphism from \mathcal{A}_3 to \mathcal{A}_2 . The square of \mathcal{A}_2 is depicted on Figure 2a; and, a surjective homomorphism from it to \mathcal{A}_3 is depicted on Figure 2b. Thus \mathcal{A}_3 and \mathcal{A}_2 are equivalent w.r.t. $\{\exists, \forall, \wedge\}$ -FO. One can also check that \mathcal{A}_2 is minimal and is therefore a Q-core of \mathcal{A}_3 , and a *posteriori* of \mathcal{A}_4 .

The behaviour of the Q-core differs from its cousins the core and the U -X-core.

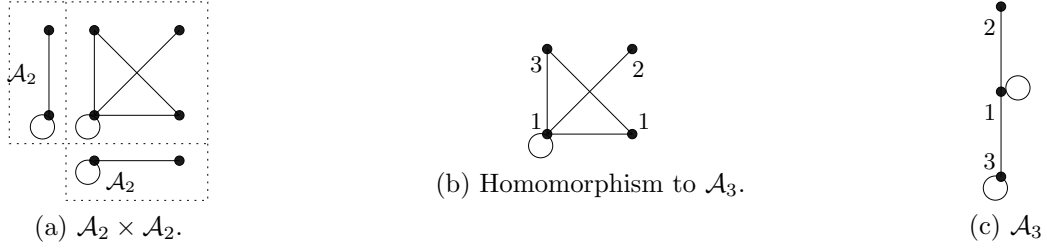


Figure 2: Surjective homomorphism from a power.

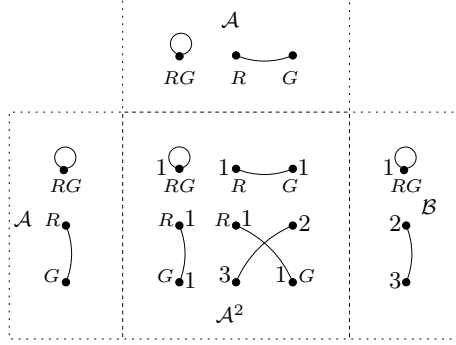


Figure 3: Example of two distinct 3-element structures (signature, E binary and two unary predicates R and G) that are equivalent w.r.t. $\{\exists, \forall, \wedge\}$ -FO.

Proposition 2. *The Q -core of a 3-element structure \mathcal{A} is not always an induced substructure of \mathcal{A} .*

Proof. Consider the signature $\sigma := \langle E, R, G \rangle$ involving a binary relation E and two unary relations R and G . Let \mathcal{A} and \mathcal{B} be structures with domain $\{1, 2, 3\}$ with the following relations.

$$\begin{aligned} E^{\mathcal{A}} &:= \{(1, 1), (2, 3), (3, 2)\} & R^{\mathcal{A}} &:= \{1, 2\} & G^{\mathcal{A}} &:= \{1, 3\} \\ E^{\mathcal{B}} &:= \{(1, 1), (2, 3), (3, 2)\} & R^{\mathcal{B}} &:= \{1\} & G^{\mathcal{B}} &:= \{1\} \end{aligned}$$

Since \mathcal{B} is a substructure of \mathcal{A} , we have $\mathcal{B} \twoheadrightarrow \mathcal{A}$. Conversely, the square of \mathcal{A}^2 contains an edge that has no vertex in the relation R and G , which ensures that $\mathcal{A}^2 \not\rightarrow \mathcal{B}$ (see Figure 3). Observe also that no two-element structure \mathcal{C} , and *a fortiori* no two-element substructure of \mathcal{A} agrees with them on $\{\exists, \forall, \wedge\}$ -FO. Indeed, if a structure \mathcal{C} agrees on $\{\exists, \forall, \wedge\}$ -FO with \mathcal{B} , it agrees also on $\{\exists, \wedge\}$ -FO. Thus, the core of \mathcal{B} is also the core of \mathcal{C} and must appear as an induced substructure of \mathcal{C} . This core is the one-element substructure of \mathcal{B} induced by 1. In order to have a surjective homomorphism from a power of \mathcal{C} to \mathcal{B} , this power must contain a non-loop, and so does \mathcal{C} . This non-loop must in \mathcal{C} be adjacent to another vertex (this is a $\{\exists, \forall, \wedge\}$ -FO-expressible property that holds in $\mathcal{B} \forall x \exists y E(x, y)$). The structure \mathcal{C} would therefore be a two element structure satisfying

$$E^{\mathcal{C}} \subseteq \{(1, 1), (1, 2), (2, 1)\} \quad R^{\mathcal{C}} \subseteq \{1\} \quad G^{\mathcal{C}} \subseteq \{1\}$$

A power of \mathcal{C} would therefore be connected, which is not the case of \mathcal{B} , preventing the existence of any surjective homomorphism. \square

We do not know whether the Q -core of a structure is unique. We will explore in the following section Q -cores over some special classes and show that it behaves well in these cases.

5 Q-cores over classes

5.1 The Boolean case

A Boolean structure \mathcal{B} has domain $B := \{0, 1\}$. The results of this section apply to arbitrary (not necessarily finite) signatures. We give the following lemma ultimately for illustrative purposes (the gist of its proof will be reused several times). The *pH-type* $T(b)$ of $b \in \mathcal{B}$ is the set of all formulae $\varphi(x)$ in one free variable x from $\{\exists, \forall, \wedge\}$ -FO such that $\mathcal{B} \models \varphi(x)$ (pH stands for positive Horn).

Lemma 4. *If \mathcal{B} is a Boolean structure such that the pH-types $T(0)$ and $T(1)$ in \mathcal{B} coincide, then \mathcal{B} has an automorphism swapping 0 and 1.*

Proof. Suppose there is no such automorphism, then w.l.o.g. we may assume there exists a conjunction of atoms $\theta(x, y)$, involving only variables x and y , such that $\mathcal{B} \models \theta(0, 1)$ but $\mathcal{B} \not\models \theta(1, 0)$. Now, $\mathcal{B} \models \theta(0, 0)$ iff $\mathcal{B} \models \theta(1, 1)$, since 0 and 1 are of the same pH-type. If $\mathcal{B} \models \theta(0, 0)$ then $\mathcal{B} \models \forall x \theta(x, 0)$ but $\mathcal{B} \not\models \forall x \theta(x, 1)$ (contradiction). Similarly, if $\mathcal{B} \not\models \theta(0, 0)$ then $\mathcal{B} \models \exists x \theta(0, x)$ but $\mathcal{B} \not\models \exists x \theta(1, x)$ (contradiction). \square

Theorem 4. *Let \mathcal{A} and \mathcal{B} be Boolean structures that are equivalent w.r.t. $\{\exists, \forall, \wedge\}$ -FO. Then \mathcal{A} and \mathcal{B} are isomorphic.*

Proof. We consider the pH-types $T^{\mathcal{A}}(0)$ and $T^{\mathcal{A}}(1)$ of 0 and 1 in \mathcal{A} , respectively (likewise with \mathcal{B} superscripts for \mathcal{B}).

Case I. $T^{\mathcal{A}}(0) = T^{\mathcal{A}}(1)$. It follows that $T^{\mathcal{A}}(0) = T^{\mathcal{A}}(1) = T^{\mathcal{B}}(0) = T^{\mathcal{B}}(1)$, since $\varphi(x) \in T^{\mathcal{A}}(0)$ iff $\mathcal{A} \models \forall x \varphi(x)$ iff $\mathcal{B} \models \forall x \varphi(x)$ iff $\theta(x) \in T^{\mathcal{B}}(0)$ etc. In this case the function $A \rightarrow B$ given by $0 \mapsto 0$ and $1 \mapsto 1$ is an isomorphism, as in the proof of Lemma 4. (Of course, $0 \mapsto 1$ and $1 \mapsto 0$ is also an isomorphism.)

Case II. $T^{\mathcal{A}}(0)$ and $T^{\mathcal{A}}(1)$ are incomparable. Let $\theta_0(x)$ be in $T^{\mathcal{A}}(0)$ but not in $T^{\mathcal{A}}(1)$; and let $\theta_1(x)$ be in $T^{\mathcal{A}}(1)$ but not in $T^{\mathcal{A}}(0)$. Let $z(0)$ be the witness of $\exists x \theta_0(x)$ in \mathcal{B} ; and let $z(1)$ be the witness of $\exists x \theta_1(x)$ in \mathcal{B} . Since $\mathcal{A} \not\models \exists x \theta_0(x) \wedge \theta_1(x)$, $\mathcal{B} \not\models \exists x \theta_0(x) \wedge \theta_1(x)$ and $z(0) \neq z(1)$. We claim $z(0 \mapsto z(0), 1 \mapsto z(1))$ is an isomorphism from \mathcal{A} to \mathcal{B} . If not, then w.l.o.g. we may assume there exists an atom (maybe with variables identified) $\theta(x, y)$ such that $\mathcal{A} \models \theta(0, 1)$ but $\mathcal{B} \not\models \theta(z(0), z(1))$. Now, $\mathcal{A} \models \theta(0, 0)$ iff $\mathcal{A} \models \theta_0(0) \wedge \theta(0, 0)$ iff $\mathcal{A} \models \exists x \theta_0(x) \wedge \theta(x, x)$ iff $\mathcal{B} \models \exists x \theta_0(x) \wedge \theta(x, x)$ iff $\mathcal{B} \models \theta(z(0), z(0))$. The proof is completed as in that of Lemma 4.

Case III. W.l.o.g. $T^{\mathcal{A}}(0) \subseteq T^{\mathcal{A}}(1)$ but $T^{\mathcal{A}}(0) \neq T^{\mathcal{A}}(1)$. Let $\theta_1(x)$ be in $T^{\mathcal{A}}(1)$ but not in $T^{\mathcal{A}}(0)$. Let $z(1)$ be the witness of $\exists x \theta_1(x)$ in \mathcal{B} . $z(1)$ is unique since $\mathcal{B} \not\models \forall x \theta_1(x)$. Let $z(0)$ be the other element of \mathcal{B} . We claim z is an isomorphism from \mathcal{A} to \mathcal{B} . If not, then there exists a conjunction of atoms $\theta(x, y)$ such that (we lose the w.l.o.g.) either $\mathcal{A} \models \theta(0, 1)$ but $\mathcal{B} \not\models \theta(z(0), z(1))$, or $\mathcal{B} \models \theta(0, 1)$ but $\mathcal{A} \not\models \theta(z(0), z(1))$. In fact, we can still deal with both cases at once, since $\mathcal{A} \models \theta(1, 1)$ iff $\mathcal{A} \models \theta_1(1) \wedge \theta(1, 1)$ iff $\mathcal{A} \models \exists x \theta_1(x) \wedge \theta(x, x)$ etc. and $\mathcal{B} \models \theta(1, 1)$. The proof concludes as in Lemma 4. \square

In the extended logic $\{\exists, \forall, \wedge, =\}$ -FO, it follows that every structure of size at most 2 satisfies the ideal of core. For $\{\exists, \forall, \wedge\}$ -FO we can only say the following.

Proposition 3. *Every Boolean structure \mathcal{B} is either a Q-core, or its Q-core is the substructure induced by either of its elements. In particular, the Q-core of \mathcal{B} is unique up to isomorphism and is an induced substructure of \mathcal{B} .*

Proof. If \mathcal{B} generates the same QCSP as a one-element structure \mathcal{A} with domain $\{0\}$, then it is clear that the pH-types $T^{\mathcal{B}}(0)$, $T^{\mathcal{B}}(1)$ and $T^{\mathcal{A}}(0)$ coincide. This gives uniqueness and induced substructure in this case. Otherwise, the only possibility – to violate the statement – is for \mathcal{B} to have as Q-core a non-induced substructure. But this is impossible by Theorem 4. \square

Lemma 4 does not extend to structures of size three. There exists \mathcal{H}_1 of size three such that every element of \mathcal{H}_1 has the same pH-type and yet \mathcal{H}_1 has no non-trivial automorphism ($H_1 := \{0, 1, 2\}$ and $E^{\mathcal{H}_1} := \{(0, 0), (1, 1), (2, 2), (1, 2)\}$). However, \mathcal{H}_1 is not a Q-core.

5.2 Unary structures

Let σ be a fixed relational signature that consists of n unary relation symbols M_1, M_2, \dots, M_n . A structure over such a signature is deemed *unary*.

Let w be a string of length n over the alphabet $\{0, 1\}$. We write $w(x)$ as an abbreviation for the quantifier-free formula $\bigwedge_{1 \leq i \leq n, w[i]=1} M_i(x)$. Each element a of a unary structure \mathcal{A} corresponds to a word w , which is the largest word bitwise such that $\mathcal{A} \models w(x/a)$. Let w_\forall be the bitwise \wedge of the words associated to each element. The unary structure \mathcal{A} satisfies the *canonical universal sentence* $\forall y w_\forall(y)$ (note that w_\forall is also the largest word bitwise among such satisfied universal formulae).

Proposition 4. *The Q-core of a unary structure \mathcal{A} is the unique substructure of \mathcal{A} defined as follows. The Q-core of \mathcal{A} is the core \mathcal{A}' of \mathcal{A} if they share the same canonical universal sentence and the disjoint union of \mathcal{A}' with a single element corresponding to w_\forall where $\forall y w_\forall(y)$ is the canonical universal sentence of \mathcal{A} .*

Proof. A positive Horn sentence over a unary signature is logically equivalent to a conjunction of formulae that do not share any variables. Each conjunct is either a universal formulae of the form $\forall y w(y)$ or an existential formulae of the form $\exists x w(x)$.

The core \mathcal{A}' is a substructure of the Q-core, so we need only enforce that the Q-core and \mathcal{A}' satisfy the same canonical universal sentence. This is achieved with the optional addition of an element corresponding to w_\forall where $\forall y w_\forall(y)$ is the canonical universal sentence of \mathcal{A} . \square

5.3 Structures with an isolated element

We say that a pH-sentence is a *proper pH-sentence*, if it has at least one universally quantified variable x_1 that occurs in some atom in the quantifier-free part. Generally, we will say that a sentence is *proper* if any variable x_1 occurs in some atom and we will be always working with such sentences unless otherwise stated (otherwise, we would simply discard x_1 and consider the equivalent sentence with one less variable). We will say that a proper pH-sentence ψ induced from a proper pH-sentence φ by the removal of some conjuncts is a *proper subsentence* of ψ .

Let σ be a signature that consists of finitely many relation symbols R_i of respective arity r_i . We will consider the set of minimal proper pH-sentences w.r.t. σ , that is all formulae of the form $\forall x_1 \exists x_2 \dots \exists x_{r_i} R_i(\bar{x})$, where the tuple \bar{x} is a permutation of the variables x_1, x_2, \dots, x_{r_i} where x_1 has been transposed with some other variable. There are $r(\sigma) = \sum_{R_i \in \sigma} r_i$ such formulae.

Theorem 5. *Let \mathcal{A} be a σ -structure. The following are equivalent.*

1. \mathcal{A} does not satisfy any proper pH-sentence.

2. \mathcal{A} does not satisfy any of the $r(\sigma)$ minimal proper pH-sentences w.r.t. σ .
3. $\mathcal{A}^{r(\sigma)}$ contains an isolated element.

Proof. The first point implies trivially the second. We show the converse. Note that any proper pH-sentence φ contains as a proper subinstance a sentence of the form $Q_1x_1Q_2x_2\ldots\forall x_j\ldots Q_rx_r R(\bar{x})$, where the Q_i represent some arbitrary quantifiers. By assumption, the structure \mathcal{A} models $\exists x_j\forall x_1\forall x_2\ldots\forall x_r\neg R(\bar{x})$. Thus, it follows that \mathcal{A} models the weaker sentence $\forall x_1\forall x_2\ldots\exists x_j\ldots\forall x_r\neg R(\bar{x})$ (the same strategy for selecting a witness for x_j will work) and the even weaker sentence where some universal quantifiers are turned to existential ones, namely those for which Q_j is universal (the strategy for these new existential variable can be chosen arbitrarily). So, \mathcal{A} does not model the negation of this last sentence which is $Q_1x_1Q_2x_2\ldots\forall x_j\ldots Q_rx_r R(\bar{x})$, which is a subinstance of φ . By monotonicity, \mathcal{A} does not model φ either.

We now prove that the second point implies the third. Let φ_i be the i th minimal proper pH-sentence w.r.t. σ . Let a_i be a witness for the unique existential variable of $\neg\varphi_i$ that \mathcal{A} does not satisfy φ_i . It is a simple exercise to check that $(a_1, a_2, \ldots, a_{r_i})$ is an isolated element of $\mathcal{A}^{r(\sigma)}$.

Conversely, if $\bar{a} := (a_1, a_2, \ldots, a_{r_i})$ is an isolated element of $\mathcal{A}^{r(\sigma)}$ then \bar{a} is a witness that $\mathcal{A}^{r(\sigma)}$ does not satisfy any minimal proper pH-sentence φ_i . Consequently, there exists some a_{j_i} witnessing that \mathcal{A} does not satisfy φ_i and we are done. \square

Example 5. In the case of directed graphs, the minimal proper pH-sentences are $\forall x_1\exists x_2 E(x_1, x_2)$ and $\forall x_1\exists x_2 E(x_2, x_1)$. A directed graph which does not satisfy them will satisfy their negation $\exists x_1\forall x_2\neg E(x_1, x_2)$ and $\exists x_1\forall x_2\neg E(x_2, x_1)$. A witness for the existential x_1 in the first sentence will be a *source*, and in the second sentence a *sink*, respectively.

So a directed graph has a source and a sink if, and only if, it does not satisfy any proper pH-sentence, if and only if, its square has an isolated element.

Corollary 2. *The Q-core of a structure \mathcal{A} that does not satisfy any proper pH-sentence is the unique substructure of \mathcal{A} may be found as follows. The Q-core of \mathcal{A} is the core \mathcal{A}' of \mathcal{A} , if $\mathcal{A}^{r(\sigma)}$ contains an isolated element, and the disjoint union of \mathcal{A}' and an isolated element, otherwise.*

Proof. By assumption \mathcal{A} does not satisfy any proper pH-sentence. Consequently a minimal structure \mathcal{A}' (both w.r.t. domain size and number of tuples) which satisfies the same pH-sentences as \mathcal{A} will satisfy the same pp-sentences as \mathcal{A} and none of the proper pH-sentences either. It follows that \mathcal{A}' must contain the core of \mathcal{A} (and can be no smaller). If this core satisfies no proper pH-sentence then we are done and by the previous theorem $\mathcal{A}^{r(\sigma)}$ has an isolated element. Otherwise, we must look for a structure that contains the core of \mathcal{A} and does not satisfy any proper universal sentence. Adding tuples to \mathcal{A} can clearly not force this property by monotonicity of QCSP. Thus, the minimal (and unique) such structure will be obtained by the addition of an isolated element. Note that in this second case we have also a substructure of \mathcal{A} . \square

Remark 1. It follows that checking whether a structure with an isolated element is a Q-core is of the same complexity as checking whether it is a core. Recall that the latter is known to be a co-NP-complete decision problem (the induced sub-structure that ought to be a core is given via an additional monadic predicate M), see [11]. We show that the former is also co-NP-complete (we also assume a monadic predicate as in this particular case the Q-core is an induced substructure), by showing inter-reducibility of both problem.

(hardness) Let $\langle \mathcal{A}, M \rangle$ be the input to the core problem (we assume that it is not trivial and that M does not contain any isolated element). If $\mathcal{A}^{r(\sigma)}$ has an isolated element (it can be done

in polynomial time as $r(\sigma)$ does not depend on \mathcal{A}) then we reduce to $\langle \mathcal{A}, M \rangle$, and to $\langle \tilde{\mathcal{A}}, \tilde{M} \rangle$ otherwise, where $\tilde{\mathcal{A}}$ consists of the disjoint union of \mathcal{A} with an isolated element and \tilde{M} is the union of M with this new element.

(co-NP-complete algorithm) Let $\langle \tilde{\mathcal{A}}, \tilde{M} \rangle$ be the input to the Q-core problem such that $\tilde{\mathcal{A}}$ has an isolated element. We check whether the alleged Q-core (the substructure of $\tilde{\mathcal{A}}$ induced by \tilde{M}) elevated to the r th power has an isolated element. If it does not we answer no. If the alleged Q-core has more than one isolated element we answer also no. Otherwise, we remove at most one isolated element from \tilde{M} to derive $M \subseteq \tilde{M}$ and reduce to the core question w.r.t. $\langle \tilde{\mathcal{A}}, M \rangle$.

6 The usefulness of Q-cores

Graphs are relational structures with a single symmetric relation E . We term them *partially reflexive* (p.r.) to emphasise that any vertex may or may not have a self-loop. A *p.r. tree* may contain self-loops but no larger cycle C_n for $n \geq 3$. A *p.r. pseudotree* contains at most one cycle C_n for $n \geq 3$. A *p.r. forest* (resp., *pseudoforest*) is the disjoint union of p.r. trees (resp., p.r. pseudotrees).

Since p.r. forests (resp., pseudoforests) are closed under substructures, we can be assured that a Q-core of a p.r. forest (resp., pseudoforest) is a p.r. forest (resp., pseudoforest). It is clear from inspection that the Q-core of p.r. forest (resp., pseudoforest, p.r. cycle) is unique up to isomorphism, but we do not prove this as it does not shed any light on the general situation. The doubting reader may substitute “a/ all” for “the” in future references to Q-cores in this section.

The complexity classifications of [14] were largely derived using the properties of equivalence w.r.t. $\{\exists, \forall, \wedge\}$ -FO. This will be the central justification for the following propositions.

Let \mathcal{K}_i^* and \mathcal{K}_i be the reflexive and irreflexive i -cliques, respectively. Let $[n] := \{1, \dots, n\}$. For $i \in [n]$ and $\alpha \in \{0, 1\}^n$, let $\alpha[i]$ be the i th entry of α . For $\alpha \in \{0, 1\}^*$, let \mathcal{P}_α be the path with domain $[n]$ and edge set $\{(i, j) : |j - i| = 1\} \cup \{(i, i) : \alpha[i] = 1\}$. For a tree \mathcal{T} and vertex $v \in T$, let $\lambda_{\mathcal{T}}(v)$ be the shortest distance in \mathcal{T} from v to a looped vertex (if \mathcal{T} is irreflexive, then $\lambda_{\mathcal{T}}(v)$ is always infinite). Let $\lambda_{\mathcal{T}}$ be the maximum of $\{\lambda_{\mathcal{T}}(v) : v \in T\}$. A tree is *loop-connected* if the self-loops induce a connected subtree. A tree \mathcal{T} is *quasi-loop-connected* if either 1.) it is irreflexive, or 2.) there exists a connected reflexive subtree \mathcal{T}_0 (chosen to be **maximal**) such that there is a walk of length $\lambda_{\mathcal{T}}$ from every vertex of \mathcal{T} to \mathcal{T}_0 .

6.1 Partially reflexive forests

It is not true that, if \mathcal{H} is a p.r. forest, then either \mathcal{H} admits a majority polymorphism, and $\text{QCSP}(\mathcal{H})$ is in NL, or $\text{QCSP}(\mathcal{H})$ is NP-hard. However, the notion of Q-core restores a clean delineation.

Proposition 5. *Let \mathcal{H} be a p.r. forest. Then either the Q-core of \mathcal{H} admits a majority polymorphism, and $\text{QCSP}(\mathcal{H})$ is in NL, or $\text{QCSP}(\mathcal{H})$ is NP-hard.*

Proof. We assume that graphs have at least one edge (otherwise the Q-core is \mathcal{K}_1). Irreflexive forests are a special case of bipartite graphs, which are all equivalent w.r.t. $\{\exists, \forall, \wedge\}$ -FO, their Q-core being \mathcal{K}_2 when they have no isolated vertex (see example 3) and $\mathcal{K}_2 + \mathcal{K}_1$ otherwise.

We assume from now on that graphs have at least one edge and one self-loop. The one vertex case is \mathcal{K}_1^* . We assume larger graphs from now on. If the graph contains an isolated element then its Q-core is $\mathcal{K}_1 + \mathcal{K}_1^*$. Assume from now on that the graph does not have an isolated element.

We deal with the disconnected case first. If the graph is reflexive, then its Q-core is $\mathcal{K}_1^* + \mathcal{K}_1^*$. Otherwise, the graph is properly partially reflexive in the sense that it embeds both \mathcal{K}_1^* and \mathcal{K}_1 . If the graph has an irreflexive component then its Q-core is $\mathcal{K}_2 + \mathcal{K}_1^*$. If the graph has no irreflexive component, then its Q-core is $\mathcal{K}_1^* + \mathcal{P}_{10^\lambda}$ where λ is the longest walk from any vertex to a self-loop. To see this last case gives an equivalent QCSP, we may consider power surjective homomorphisms, together with the fact that the Q-core must not satisfy $\forall x \exists y_1, \dots, y_{\lambda-1} E(x, y_1) \wedge E(y_1, y_2) \wedge \dots \wedge E(y_{\lambda-2}, y_{\lambda-1})$.

We now follow the classification of [14]. If a p.r. forest contains more than one p.r. tree, then the Q-core is among those formed from the disjoint union of exactly two (including the possibility of duplication) of \mathcal{K}_1 , \mathcal{K}_1^* , \mathcal{P}_{10^λ} , \mathcal{K}_2 . Each of these singularly admits a majority polymorphism, therefore so does any of their disjoint unions.

We now move on to the connected case, i.e. it remains to consider p.r. trees \mathcal{T} . If \mathcal{T} is irreflexive, then its Q-core is \mathcal{K}_2 or \mathcal{K}_1 , which admit majority polymorphisms. If \mathcal{T} is loop-connected, then it admits a majority polymorphism [14]. If \mathcal{T} is quasi-loop-connected, then it is QCSP-equivalent to one of its subtrees that is loop-connected [14] which will be its Q-core. In all other cases $\text{QCSP}(\mathcal{T})$ is NP-hard, and \mathcal{T} does not admit majority [14]. \square

6.2 Irreflexive Pseudoforests

A *pseudotree* is a graph that involves at most one cycle. A *pseudoforest* is the disjoint union of a collection of pseudotrees.

Proposition 6. *Let \mathcal{H} be an irreflexive pseudoforest. Then either the Q-core of \mathcal{H} admits a majority polymorphism, and $\text{QCSP}(\mathcal{H})$ is in NL, or $\text{QCSP}(\mathcal{H})$ is NP-hard.*

Proof. We follow the classification of [15]. If \mathcal{H} is bipartite, then its Q-core is either \mathcal{K}_2 , \mathcal{K}_1 , $\mathcal{K}_2 + \mathcal{K}_1$ (see [6]) and this admits a majority polymorphism. Otherwise its Q-core contains an odd cycle, which does not admit a majority polymorphism, and $\text{QCSP}(\mathcal{H})$ is NP-hard. \square

7 Computing a Q-core

We may use Theorem 2 to provides a first algorithm (Algorithm 1). This does not appear very promising if we wish to use Q-cores as a preprocessing step. We will propose and illustrate a general and less naive method to compute Q-cores by computing U - X -core and cores first.

Another nice feature of cores and U - X -cores which implies their uniqueness is the following: any substructure \mathcal{C} of \mathcal{A} that agrees with it on $\{\exists, \wedge\}$ -FO (respectively on $\{\exists, \forall, \wedge, \vee\}$ -FO) will contain the core (respectively the U - X -core). Consequently, the core and the U - X -core may be computed in a *greedy fashion*. Assuming that the Q-core would not satisfy this nice property, why should this concern the Q-core? Well, we know that **any** Q-core will lie somewhere between the U - X -core and the core that are induced substructures: this is a direct consequence of the inclusion of the corresponding fragments of first-order logic and their uniqueness. Moreover, according to our current knowledge, checking for equivalence appears, at least on paper, much easier for $\{\exists, \forall, \wedge, \vee\}$ -FO than $\{\exists, \forall, \wedge\}$ -FO: compare the number of functions from A to the power set of B ($2^{|B|^{|A|}} = 2^{|B| \times |A|}$) with the number of functions from A^r to B ($|B|^{|A|^r}$) where r could be as large as $|A|^{|B|}$ and can certainly be greater than $r \approx |A|$ (see Proposition 1). So it make sense to bound the naive search for Q-cores.

Algorithm 1: A naive approach to compute the Q-cores.

input : A structure \mathcal{A}
output : The list L of Q-cores of \mathcal{A}
initialisation: set $L := \{\mathcal{A}\}$
forall the substructure \mathcal{B} of \mathcal{A} do
 if *there exists a surjective homomorphism from $\mathcal{A}^{|A||B|}$ to \mathcal{B}* **then**
 if *there exists a surjective homomorphism from $\mathcal{B}^{|B||A|}$ to \mathcal{A}* **then**
 Remove any structure containing \mathcal{B} in L ;
 Add \mathcal{B} to L ;
 end
 end
end
output : List of Q-cores L

Furthermore, we know that the U - X -core can be identified by specific surjective hypermorphisms that act as the identity on X and contain the identity on U [13] which makes the search for the U - X -core somewhat easier than its definition suggest (see Algorithm 2).

Observe also that X must contain the core \mathcal{C} of the U - X -core \mathcal{B} , which is also the core of the original structure \mathcal{A} (this is because h induces a so-called retraction of \mathcal{A} to the substructure $\mathcal{A}|_X$ induced by X). Thus we may compute the core greedily from X . Next, we do a little bit better than using our naive algorithm, by interleaving steps where we find a substructure that is $\{\exists, \forall, \wedge\}$ -FO-equivalent, with steps where we compute its U - X -core (one can find a sequence of distinct substructures \mathcal{B} , \mathcal{D} and \mathcal{B}' such that \mathcal{B} is a U - X -core, which is $\{\exists, \forall, \wedge\}$ -FO-equivalent to \mathcal{D} , whose U - X -core \mathcal{B}' is strictly smaller than \mathcal{B} , see Example 6). Algorithm 3 describes this proposed method informally when we want to compute **one** Q-core (of course, we would have no guarantee that we get the smallest Q-core, unless the Q-core can be also greedily computed, which holds for all cases we have studied so far).

In Algorithm 3, we have purposely not detailed line ???. We could use the characterisation of $\{\exists, \forall, \wedge\}$ -FO-containment via surjective homomorphism from a power of Theorem 3 as in Algorithm 1. Alternatively, we can use a refined form of (iii) in this Theorem and use the canonical sentences in Π_2 -form $\psi_{\mathcal{B}, m_1}$ and $\psi_{\mathcal{D}, m_2}$, with $m_1 := \min(|D|, |U|)$ and $m_2 := |U|$ (see Definition 5). The test would consist in checking that \mathcal{B} satisfies $\psi_{\mathcal{D}, m_2}$ (where we may relativise to universal variables to U and existential variables to X) and \mathcal{D} satisfies $\psi_{\mathcal{B}, m_1}$. This is correct because we know that we may relativise every universal variable to U within \mathcal{B} . Thus, it suffices to consider Π_2 -sentences with at most $|U|$ universal variables.

Example 6. We describe a run of Algorithm 3 on input $\mathcal{A} := \mathcal{A}_4$. During the initialisation, we compute its U - X -core $\mathcal{B} := \mathcal{A}_3$ and discover that $U = \{2, 3\}$ and $X = \{1, 2\}$. We compute $\mathcal{C} := \mathcal{A}_1$, the core of the substructure induced by X .

Note that $\mathcal{B} = \mathcal{A}_3$ is isomorphic to \mathcal{P}_{110} . Next the algorithm guesses a substructure \mathcal{D} of \mathcal{B} that contains \mathcal{C} : e.g. it drops the self-loop around vertex 3 to obtain a structure isomorphic to \mathcal{P}_{010} and checks successfully equivalence w.r.t. $\{\exists, \forall, \wedge\}$ -FO (there is a surjective homomorphism from \mathcal{P}_{010} to \mathcal{P}_{110} ; and, conversely we can use the surjective homomorphism from $\mathcal{P}_{110} \times \mathcal{P}_{110}$ to $\mathcal{P}_{10} \times \mathcal{P}_{11}$ composed with that from the former to \mathcal{P}_{010}).

Next the algorithm computes the U' - X' -core \mathcal{B}' of \mathcal{D} which is \mathcal{A}_2 (witnessed by $h'(1) = 1, h'(2) = h'(3) = \{1, 2, 3\}, U' := \{2\}, X' := \{1\}$) and sets $\mathcal{B} := \mathcal{B}' = \mathcal{A}_2$.

Algorithm 2: A greedy approach to compute the U - X -core.

input : a structure \mathcal{A} .
output : the U - X -core of \mathcal{A} .
variables : U and X two subsets of A .
variable : h a surj. hypermorphism from \mathcal{A} to \mathcal{A} s.t. $h(U) = A$ and $h^{-1}(X) = A$.
variable : \mathcal{B} an induced substructure of \mathcal{A} such that $B = U \cup X$.
initialisation: set $U := A$, $X := A$, $\mathcal{B} := \mathcal{A}$, h the identity
repeat
 guess a subset U' of U and a subset X' of X ;
 let h' be a map from B to B ;
 forall the x' **in** X' **do** **set** $h'(x') := \{x'\}$;
 forall the u' **in** $U' \setminus X'$ **do** **guess** x' **in** X' **set** $h'(u') := \{u', x'\}$;
 forall the z' **in** $B \setminus (U' \cup X')$ **do**
 guess x' **in** X' **set** $h(z') := \{x'\}$;
 guess u' **in** U' **set** $h(u') := h(u') \cup \{z'\}$;
 end
 if h' *is a surj. hypermorphism from B to B* **then**
 set \mathcal{B} to be the substructure of \mathcal{B} induced by $U' \cup X'$;
 set $U := U'$, $X := X'$ and $h := h' \circ h$;
 end
until U and X are minimal;
output : \mathcal{B} .

Algorithm 3: Bounded Search for a Q-core.

input : a structure \mathcal{A}
output : a Q-core \mathcal{B} of \mathcal{A}
initialisation: compute the U - X -core of \mathcal{A} as in Algorithm 2;
set \mathcal{B} to be the U - X -core;
set \mathcal{C} to be the core \mathcal{C} of the substructure of \mathcal{B} induced by X ;
repeat
 guess \mathcal{D} a substructure of \mathcal{B} that contains \mathcal{C} ;
 check that \mathcal{B} and \mathcal{C} are equivalent w.r.t. $\{\exists, \forall, \wedge\}$ -FO;
 set \mathcal{B} to be the U - X -core of \mathcal{D} ;
until \mathcal{B} is minimal;
output : \mathcal{B} .

The algorithm stops eventually and outputs \mathcal{A}_2 as it is minimal.

8 Conclusion

We have introduced a notion of Q-core and demonstrated that it does not enjoy all of the properties of cores and U - X -core. In particular, there need not be a unique minimal element w.r.t. size in the equivalence class of structures agreeing on pH-sentences. However, we suspect that the notion of Q-core we give is robust, in that the Q-core of any structure \mathcal{B} is unique up to isomorphism; and, that it sits inside any substructure of \mathcal{B} that satisfies the same sentence of $\{\exists, \forall, \wedge\}$ -FO, making it computable in a greedy fashion. Thus, the nice behaviour of Q-cores is almost restored, but “induced substructure” in the properties of core or U - X -core must be replaced by the weaker “substructure”.

Generalising the results about Q-cores of structures with an isolated element to disconnected structures is already difficult. Just as the pH-theory of structures with an isolated element is essentially determined by their pp-theory, so the pH-theory of disconnected structures is essentially determined by its $\forall\exists^*$ fragment (see [15]).

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